2010

Electronic properties of carbon nanotubes with distinct bond lengths

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Abstract

In band structure calculations commonly used to derive the electronic properties of carbon nanotubes it is generally assumed that all bond lengths are equal. However, hexagonal carbon lattices are often irregular and may contain as many as three distinct bond lengths. A regular (n,m) carbon nanotube will be metallic if p=(n-m)/3 for integer p. Here we analytically derive the generalized condition for metallic irregular carbon nanotubes. This condition is particularly relevant to small radius nanotubes and nanotubes experiencing small applied strains.

Keywords

bond, lengths, carbon, distinct, properties, nanotubes, electronic

Disciplines

Physical Sciences and Mathematics

Publication Details

Bunder, J. E. & Hill, J. M. (2010). Electronic properties of carbon nanotubes with distinct bond lengths. Journal of Applied Physics, 107 (2), 023511-1-023511-5.

Electronic properties of carbon nanotubes with distinct bond lengths

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(Received 12 August 2009; accepted 10 December 2009; published online 25 January 2010)

In band structure calculations commonly used to derive the electronic properties of carbon nanotubes, it is generally assumed that all bond lengths are equal. However, hexagonal carbon lattices are often irregular and may contain as many as three distinct bond lengths. A regular (n,m) carbon nanotube will be metallic if $p=(n-m)/3$ for integer p. Here we analytically derive the generalized condition for metallic irregular carbon nanotubes. This condition is particularly relevant to small radius nanotubes and nanotubes experiencing small applied strains.
 [doi:10.1063/1.3289320]

I. INTRODUCTION

It is well known that a real carbon nanotube (CNT) lattice, like most real lattices, is not perfectly regular.[1–5] Small deviations in bond lengths will not usually have a significant effect on the electronic properties of a lattice. However, in the case of a CNT, the electronic behavior is strongly dependent on the lattice structure so that any deviation from the ideal case will have a noticeable effect. In this paper, we derive a rule which determines when a CNT with variable bond lengths will be metallic. Variable bond lengths form naturally in CNT and are particularly noticeable in small radius nanotubes because the large curvature tends to elongate the bonds along the circumference.[6] These differences in bond lengths can be further enhanced by small applied strains.

Experimental studies show that placing a CNT under some kind of increasing strain may cause it to oscillate between conducting and semiconducting behavior.[7–12] The potential for electronic properties to be determined by mechanical means has many possible applications such as sensors and transistors. Theoretical studies of strained CNT find that the band gap will oscillate between zero and nonzero values as the strain is increased, in agreement with the experimental results.[13–19] However, most of these theoretical studies tend to assume that the CNT lattice vectors distort like solid object vectors. Here, as an example of how to apply our general rule for metallic CNT, we consider a CNT under small axial and torsional strains, where small implies that the applied strains are not sufficient to cause buckling or kinking,[20,21] while taking into account the fact that lattices do not distort like solid objects.

A regular CNT lattice is a rolled up regular hexagonal lattice which can be defined by two identical equilateral triangular lattices with lattice vectors $\mathbf{c}_1$ and $\mathbf{c}_2$, which are offset by σ_1. On rolling up the two-dimensional lattice we can define a vector $\mathbf{C}=n\mathbf{c}_1+m\mathbf{c}_2$ with integers n and m which lie along the circumference of the nanotube. The two integers (n,m) define the full range of all regular CNT structures when constrained by $n\geq m\geq 0$. When $n=m$, we have an armchair CNT, but when $m=0$, we have a zigzag CNT, while a CNT with other values of n and m are termed chiral. From simple band structure calculations, it can be shown that when $p=(n-m)/3$ is an integer, the CNT is metallic, while all other cases are semiconducting. Based on this rule, armchair CNT are always metallic, while zigzag and chiral CNT are mostly semiconducting but sometimes metallic.

Clearly the $p=(n-m)/3$ rule is not valid if the CNT is under some applied strain which distorts the lattice vectors. Numerical results also show that it is not valid when the CNT radius is small, for example, (4,0) and (5,0) are metallic[22,23] although they do not have integer p. The discrepancy is partly due to the large curvature, which distorts the bonds and hybridization effects which influence the hopping strength about the CNT circumference. However, the electronic properties of CNT are not solely determined by their geometry. Electron-electron interactions, such as Coulomb or spin interactions, are also important, particularly in small radius CNT. Here we will only briefly discuss electron-electron interactions and we will assume that interaction effects are not large and remain fairly constant during CNT distortions, so that one can easily observe how lattice distortions effect the band gap.

II. THE MODEL

A real CNT lattice, although not always regular, is reasonably well defined by three nearest neighbor vectors $\sigma_{1,2,3}$ (Refs. 1–6) with different magnitudes, as shown in Fig. 1.

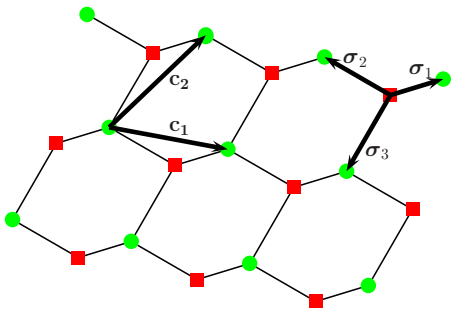

FIG. 1. (Color online) An irregular hexagonal lattice with the two sublattices represented by circles and squares.

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We can define two irregular triangular sublattices with lattice vectors $\mathbf{c}_1=\sigma_1-\sigma_2$, $\mathbf{c}_2=\sigma_1-\sigma_3$ and offset by σ_1. Although an irregular CNT can still be defined by (n,m) with $\mathbf{C}=n\mathbf{c}_1+m\mathbf{c}_2$, the simple $p=(n-m)/3$ rule for a metallic CNT no longer applies. Here, we will analytically derive a new rule for a metallic CNT which is applicable to irregular CNT by calculating when the band gap vanishes. This can be done by considering a simple tight-binding Hamiltonian which ignores all spin and charge interactions,

$$H_0=-\sum_{l=1}^{3}\sum_{xy\alpha}t_l[c_{2\alpha}^{\dagger}(x,y)c_{1\alpha}(x+a_l,y+b_l)+H.C.] \quad (1)$$

where t_l is the hopping strength between a general lattice site (x,y) on the second sublattice and $(x,y)+\boldsymbol{\sigma}_l$ on the first sublattice with $\boldsymbol{\sigma}_l=(a_l,b_l)$, and $H.C.$ is the Hermitian conjugate. The operators $c_{j\alpha}(\mathbf{r})$ and $c_{j\alpha}^{\dagger}(\mathbf{r})$ are annihilation and creation operators, respectively, at site $\mathbf{r}$ with the subscript j defining the sublattice and $\alpha=\uparrow,\downarrow$ defining the spin. The circles are $j=1$ and the squares are $j=2$ in Fig. 1. On rewriting the operators in terms of their momentum-space Fourier transform the Hamiltonian becomes

$$H_0=-\sum_{k_xk_y\alpha}[Ac_{2\alpha}^{\dagger}(k_x,k_y)c_{1\alpha}(k_x,k_y)+H.C.] \quad (2)$$

with $A=\Sigma_l t_l e^{ik_xa_l+ik_yb_l}$ from which the dispersion can be shown to be $E(k_x,k_y)=\pm|A|$.[14]

For the CNT to be metallic the dispersion may not be gapped at the Fermi energy $E_F=E(\mathbf{k}_F)$ and provided the CNT is undoped, $E_F=0$. After some algebra, a total of six zeros can be found for the dispersion relation, reflecting the hexagonal structure of the lattice. The zeros are at $\mathbf{k}_F=\pm(k_{xF},k_{yF})$ where

$$k_{xF}=[(b_k-b_i)\theta_k+(b_j-b_i)\theta_j]/d,$$

$$k_{yF}=[(a_i-a_k)\theta_k+(a_i-a_j)\theta_j]/d, \quad (3)$$

with cyclic permutations of $(i,j,k)=(1,2,3)$, $d=a_1(b_3-b_2)+a_2(b_1-b_3)+a_3(b_2-b_1)$ and $\theta_k=\cos^{-1}(t_k^2-t_i^2-t_j^2)/2t_it_j$. These angles describe the external angles of a triangle and $\theta_1+\theta_2+\theta_3=2\pi$. The lengths of the sides of this triangle are the hopping strengths $t_{1,2,3}$. Therefore, the three hopping strengths must satisfy the triangle inequality $|t_j-t_k|\le t_i\le|t_j+t_k|$ for any $(i,j,k)=(1,2,3)$. The triangle inequality condition is simply where $E(\mathbf{k})=0$ has a real solution and in the well-studied case of $t_1=t_2=t$ and $t_3=t_\perp$ it reduces to $t_\perp\le\sqrt{2}t$.[24] Note that the triangle constructed with external angles $\theta_{1,2,3}$ and sides $t_{1,2,3}$ is not related to any triangle which can be constructed on the physical lattice shown in Fig. 1 but is simply a mathematical construct which arises through the cosine relationship between $\theta_{1,2,3}$ and $t_{1,2,3}$.

On rolling the hexagonal lattice into a CNT, we define the y axis to be along the tube's axis while the x axis wraps around the tube. The x component of $\mathbf{C}$ is the circumference C and the y component is zero. The momentum along the x axis must be quantized by $k_x=2\pi p/C$ for integer p. If this quantized k_x may equal the x component of the Fermi momentum k_{xF} then the CNT is gapless and can be described as metallic. We find that a CNT is metallic when p is an integer and

$$p=\begin{cases}\pm[n\theta_3-m\theta_2]/2\pi,\\ \pm[m\theta_1+(n+m)\theta_3]/2\pi,\\ \mp[(n+m)\theta_2+n\theta_1]/2\pi.\end{cases} \quad (4)$$

Given that the θ's sum to 2π, if one solution for p is an integer, then all solutions for p are integers. When $t_1=t_2=t_2$, which is usually the case in regular CNT without very small radii, the above rule reduces to $p=(n-m)/3$.

The condition in Eq. (4) is able to account for any value of $\sigma_{1,2,3}$ and $t_{1,2,3}$ and as such can account for curvature effects which both distort the lattice vectors about the x axis,[6] and cause hybridization of π orbitals, effecting hopping around the circumference but not hopping which is predominantly in the longitudinal direction.[25,26] In a regular armchair CNT, for example, the symmetry of the lattice ensures that we always have $t_2=t_3$ and Eq. (4) shows that the armchair CNT is always metallic. In a regular zigzag CNT, however, symmetry will ensure that $t_1=t_2$ but due to hybridization $|t_3-t_1|\sim 1/n^2$, which may create a small band gap, even when the CNT satisfies $p=(n-m)/3$.[24,26] Although curvature effects do influence the size of the band gap, particularly in small radius CNT, a far greater effect is caused by electron-electron interactions.

Recently, it has been shown experimentally that ultraclean armchair CNT are in fact insulators,[27] in contradiction to Eq. (4), which predicts that a regular armchair CNT should always be metallic, even when curvature effects are taken into account. The inclusion of electron-electron interactions into the theory appears to resolve this discrepancy, resulting in an insulating armchair CNT with a band gap of the correct order.[24,27] Although the presence of electron-electron interactions may prevent a CNT from being truly metallic, it can be shown that some interaction of strength V is reduced to an effective interaction of V/n once the delocalization of the electrons about the circumference is taken into account.[24,28,29] Therefore, this effective interaction may be generally regarded as weak, provided the radius of the CNT is not small. An alternative way of reducing interactions, and one which will work for a CNT of any radius, is through screening by, for example, placing the CNT near a metallic plate or within a CNT bundle.[30,31] Therefore, despite neglecting electron-electron interactions, there are several realistic situations in which Eq. (4) is a reasonable approximation.

III. CNTS UNDER STRAIN

To illustrate Eq. (4), we consider a CNT under small torsional and longitudinal strains while assuming that the unstrained CNT is regular. The force is applied by fixing one end of the CNT and then either pulling or twisting the other end. We assume that the strain is small so that the CNT does not buckle and the hexagons in the lattice remain identical. We also assume that the part of the band gap due to electron-electron interactions is not very large and remains fairly con-

stant while the CNT is under strain so that the effects of distortion on the band gap can still be observed.

In a regular (n,m) CNT with $\sigma_k=(a_k,b_k)$,

$$\sigma_1 = a(\sin\theta + \sqrt{3}\cos\theta, \cos\theta - \sqrt{3}\sin\theta)/2,$$

$$\sigma_2 = a(\sin\theta - \sqrt{3}\cos\theta, \cos\theta + \sqrt{3}\sin\theta)/2,$$

$$\sigma_3 = -a(\sin\theta, \cos\theta),$$

$$\cos\theta = (2n+m)/2\sqrt{n^2+nm+m^2}, \tag{5}$$

where θ is the chiral angle and a is the bond length. Once a strain is applied the lattice vectors will distort to $\sigma_l=(a_l+\delta x_l, b_l+\delta y_l)$. Initially, all hopping strengths are identical $t=t_{1,2,3}$, but they distort to $t+\delta t_{1,2,3}$. To begin with we consider distortions in the triangular sublattice defined by the sublattice vectors $\mathbf{c}_{1,2}$. The sublattice vectors are originally $\mathbf{c}_l=(c_{lx},c_{ly})$ but distort to $\mathbf{c}_l=(c_{lx}+\delta c_{lx}, c_{ly}+\delta c_{ly})$ once a strain is applied.

The changes due to strain in the original length L and circumference C of the CNT are defined by ΔL and ΔC, respectively. The circumferential vector is $\mathbf{C}=n\mathbf{c}_1+m\mathbf{c}_2=(C+\Delta C,0)$. We construct a vector $\mathbf{T}=-(n+2m)\mathbf{c}_1+(2n+m)\mathbf{c}_2$ which connects two lattice sites in the same sublattice and is perpendicular to $\mathbf{C}$ in the undistorted CNT. We define $\mathbf{T}=(T_x+\Delta T_x, T_y+\Delta T_y)$, where $T_{x,y}$ are the x and y components prior to applying strain and $\Delta T_{x,y}$ are strain dependent. We can now define all strain parameters in terms of $\mathbf{T}$ and $\mathbf{C}$. The longitudinal strain is

$$\varepsilon = \Delta L/L = \Delta T_y/T_y. \tag{6}$$

The torsional angle ϕ, which defines the twist in the CNT about its longitudinal axis, can be written as $\phi=(2\pi L/C)\tan\alpha$, where α is the angle that the vector $\mathbf{T}$ makes with the y axis after distortion,

$$\tan\alpha = \Delta T_x/(T_y+\Delta T_y). \tag{7}$$

Poisson's ratio is

$$\nu = -(\Delta C/C)/(\Delta L/L) = -T_y\Delta C/C\Delta T_y. \tag{8}$$

Using the above equations, as well as the fact that the y component of $\mathbf{C}$ is always zero, we can show that

$$\delta c_{1x} = [-3m(1+\varepsilon)\tan\alpha - (2n+m)\sqrt{3}\varepsilon\nu]/g,$$

$$\delta c_{2x} = [3n(1+\varepsilon)\tan\alpha - (n+2m)\sqrt{3}\varepsilon\nu]/g,$$

$$\delta c_{1y} = -3m\varepsilon/g,$$

$$\delta c_{2y} = 3n\varepsilon/g, \tag{9}$$

where $g=2\sqrt{n^2+nm+m^2}$. We have shown that the variation in $\mathbf{c}_{1,2}$ is uniquely defined by the parameters ε, ν, and α. However, the same is not true for the variation in $\boldsymbol{\sigma}_{1,2,3}$. In general, we can write

$$\delta x_1 = \delta x + [(n-m)(1+\varepsilon)\tan\alpha - \sqrt{3}(n+m)\nu\varepsilon]/g,$$

$$\delta x_2 = \delta x + [(n+2m)(1+\varepsilon)\tan\alpha + \sqrt{3}n\nu\varepsilon]/g,$$

$$\delta x_3 = \delta x + [-(2n+m)(1+\varepsilon)\tan\alpha + \sqrt{3}m\nu\varepsilon]/g,$$

$$\delta y_1 = \delta y + (n-m)\varepsilon/g,$$

$$\delta y_2 = \delta y + (n+2m)\varepsilon/g,$$

$$\delta y_3 = \delta y - (2n+m)\varepsilon/g, \tag{10}$$

where δx and δy are to be determined.

If we set $\delta x=\delta y=0$, we can write all distortions as $\delta x_l=b_l(1+\varepsilon)\tan\alpha-\nu\varepsilon a_l$ and $\delta y_l=b_l\varepsilon$, which have been used previously in some theoretical calculations.[13–15] While this simplification is valid for specific cases, it cannot describe the general case since for longitudinal strains it incorrectly assumes that δx_l is proportional to a_l and not influenced by b_l. However, in an armchair CNT, for example, σ_1 lies along the x axis so intuitively we would expect a longitudinal strain to mainly influence the vectors $\sigma_{2,3}$, while having little effect on σ_1. This intuition agrees with numerical calculations[5,32] and completely contradicts $\delta x_l=-\nu\varepsilon a_l$. When considering strains in a lattice structure one cannot simply treat the lattice like a solid object, which is essentially what is being done by setting $\delta x=\delta y=0$. One case where $\delta x=\delta y=0$ is valid is a zigzag CNT under longitudinal strain as we obtain $\delta x_1=\delta x_2=-\sqrt{3}\nu\varepsilon/2$, $\delta x_3=0$, $\delta y_1=\varepsilon/2=\delta y_2=\delta y_3/2$, which are reasonable given the symmetry of the lattice. Also, for purely torsional strains ($\varepsilon=0$), for both armchair and zigzag cases, setting $\delta x=0$ is appropriate given the symmetry.

The additional symmetry of the armchair and zigzag CNT allow us to determine reasonable values of δx and δy for these two special cases, and these can be extrapolated to the general chiral cases. As discussed above, for an armchair CNT under longitudinal strain we expect $\delta x_1=0$ which will require $\delta x=\nu\varepsilon$, but for a zigzag CNT $\delta x=0$. Therefore, we can set $\delta x=2m\sqrt{3}\nu\varepsilon/g$, which gives reasonable values for a chiral CNT. As for δy, under longitudinal strain it is reasonable to set $\delta y=0$ for both armchair and zigzag CNT as distortions along the y axis ought to be proportional to ε. For torsional strain a reasonable value for δy is less easy to determine. As $\delta y=0$ is reasonable for both zigzag and armchair CNT under torsional strain we assume that this is also the case for chiral CNT.

We will now look at some specific examples. In these examples we wish to ignore complications arising from small radius CNT, such as curvature effects and large effective interactions, and therefore we will just consider larger radius CNT. We use Eq. (10) to determine the strain in the CNT, and then substitute the relationship[33] $t_l\propto 1/\sigma_l^2$ in Eq. (4) to determine if the CNT is metallic. Note that here, when we describe the CNT as "metallic" this description is based on band structure calculations and ignores all interaction effects. The simple relationship between the hopping strength and the bond length is accurate providing the CNT radius is not small. As discussed previously, hybridization effects increase with decreasing radius and affect hopping about the circumference, and it this which makes $t_l\propto 1/\sigma_l^2$ inaccurate for small radius CNT. It is possible to take hybridization

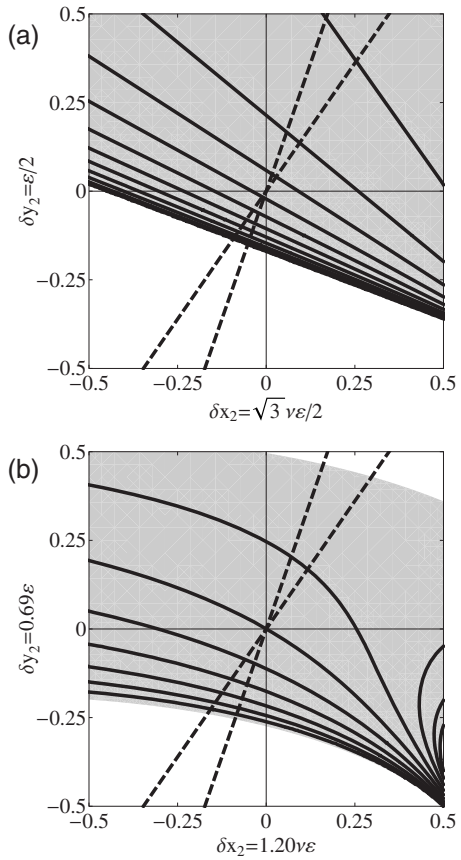

FIG. 2. Effect of longitudinal strain on (a) (25, 0) zigzag CNT and (b) (18, 6) chiral CNT. Solid lines are where the CNT is metallic, the shaded area is where the triangle inequality holds and dashed lines have gradient $1/\nu\sqrt{3}$ for $\nu=0.2$ and 0.4.

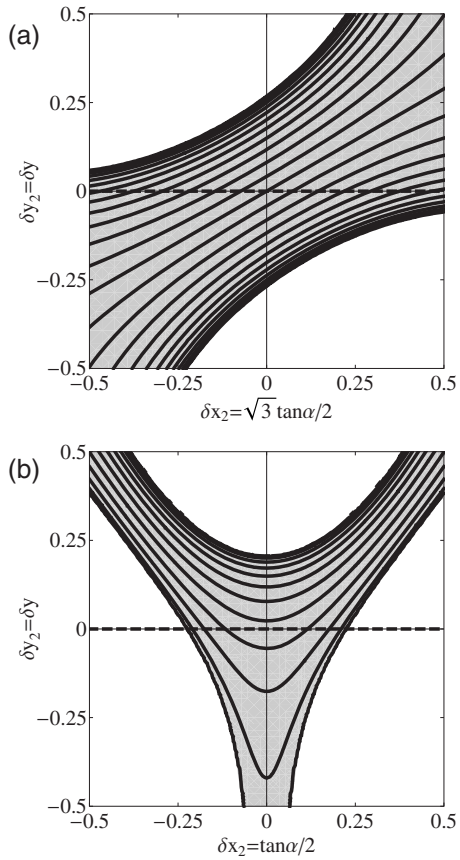

FIG. 3. Effect of torsional strain on (a) (25, 25) armchair CNT and (b) (25, 0) zigzag CNT. Solid lines are where the CNT is metallic, the shaded area is where the triangle inequality holds and dashed lines are for $\delta y=0$.

effects into account[27] but doing so would have only a minor effect as it will just slightly shift the positions of the metal-insulator transitions.

For an armchair CNT under longitudinal strain we always have $\sigma_2=\sigma_3$, and therefore $t_2=t_3$. As discussed previously, this means that an armchair is always metallic. A more interesting case is a zigzag CNT under longitudinal strain. In Fig. 2(a) we plot δx_2 against δy_2 while varying the strain ε for a (25, 0) zigzag CNT. The density of the metal-insulator transitions increases with n and therefore we have chosen n to be quite large in order to give a more detailed picture. A large value of n also has the advantage of reducing curvature effects and effective interactions. From Eq. (10) we can show that $\delta y_2=\delta x_2/\sqrt{3}\nu$ so that the actual change in the CNT with strain is represented by a straight line of gradient $1/\sqrt{3}\nu$ which passes through the origin of the δx_2 versus δy_2 contour plot. Two examples of such a line are given in Fig. 2(a) for $\nu=0.2$ and 0.4, which are reasonable values for an zigzag CNT.[32] In Fig. 2(b) we construct a similar contour plot for a (18, 6) chiral CNT. In Figs. 3 we consider a (25, 25) armchair and a (25, 0) zigzag CNT under torsional strain. The CNT are treated as classically elastic materials which maintain a constant length during torsion. As we have not fully determined δy under torsional strain, we plot for all possibilities. As before we chose large values of n because they give a greater number of metal-insulator transitions.

Although the contour plots in both Figs. 2 and 3 show a large number of metal-insulator transitions, in most single walled CNT at most only one or possibly two metal-insulator transitions will be observable before the CNT breaks. Experimental studies have shown that CNT tend to fail at approximately $\varepsilon=0.06$, although at extremely high temperatures this may be increased to $\varepsilon=2.8$.[34] For torsion, failure is at approximately $\tan\alpha=0.2-0.3$ in multiwalled CNT.[11,35] There is some evidence that it is the outermost wall of a multiwalled CNT that carries the majority of the current and torque,[11,36] and for this reason we may be able to assume that the hopping between walls is very small, relative to the hopping within the outermost wall. If this is the case then the results derived here for single walled CNT may also be applicable to multiwalled CNT. The radius of the outermost wall of a multiwalled CNT tends to be significantly larger than the radius of a typical single walled CNT and as a result the density of metal-insulator transitions is greater than what is shown in Fig. 3, allowing one to observe several metal-insulator transitions as strain increases.

The energy gap, which is the minimum of $2|E(k_x=2\pi p/C,k_y)|$ for all integer p and k_y, is directly related to the conductivity so may be experimentally verified. In Fig. 4 we plot the effects of longitudinal strain on the energy gap of five CNT with the same chirality but different radii. The change in energy gap with strain tends to be approximately linear. In general we find that all CNT with the same ratio m/n have the same gradients, but with larger radius CNT having more frequent turning points, which has the effect of

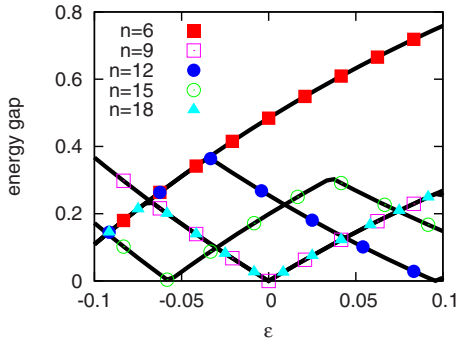

FIG. 4. (Color online) The effect of longitudinal strain on the energy gap, measured in units of hopping strength t, for $m/n=1/3$ and $\nu=0.4$.

reducing the maximum possible energy gap while possibly also increasing the number of metal insulator transitions. In addition, positive and negative gradients do not in general have the same magnitude. The slope increases with decreasing m, with armchair CNT having zero slope (since they remain metallic), and zigzag CNT having the largest. The zigzag CNT have gradients of approximately $g_+=3.58t$ and $g_-=-5t$, where t is the hopping strength of the undistorted CNT. The gradients of a CNT with any chirality can be approximated by $g_\pm(1-r)(2+6r-3r^2)/2(1+2r)$ where $r=m/n$. Previous studies have also noted a relationship between gradient and chirality,[13–15] although our different strain formulation leads to significantly larger gradients.

IV. SUMMARY

In summary, we have generalized the well-known rule $p=(n-m)/3$ for those CNT which have three distinct bond lengths. Variable bond lengths may arise naturally in all CNT and may be exaggerated by some small applied strain or by large curvature, which is particularly important in small radius nanotubes. As an example we consider a regular CNT placed under small torsional or longitudinal strains. Our results for longitudinal strains differ from previous theoretical studies. Predicting electronic properties arising from small induced strains is relevant to applications such as sensors and transistors.

ACKNOWLEDGMENTS

The support of the Australian Research Council through the Discovery Project scheme is gratefully acknowledged.

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